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# Software for Reflectivity Calculations of X-Ray Mirrors

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# Software for Reflectivity Calculations of X-Ray Mirrors*

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## ABSTRACT

With VAX software and the data libraries of Henke and Biggs-Lighthill, we have created a library of atomic scattering factors $f_1$ and $f_2$ in the energy range 0.1 keV to 10.0 keV. Scattering factor values for the elements Z = 1 to Z = 94 and in the above energy range are stored in a keyed access library (key = element symbol). This library allows one to calculate reflectivity rapidly and fold it with other components in an x-ray detector channel. Additional software allows the library data to be easily extended to higher energies. Applications have so far included KB x-ray microscopes and low energy spectrometers with mirror channels.

## SUMMARY

In recent laser fusion experiments and laser plasma interaction experiments at the Novette Laser Facility, diagnostics to measure the spatial, temporal, and spectral characteristics of x-ray emissions have formed the majority of instrumentation. An x-ray detector channel may contain any of the following components (Figure 1):

a. thin foil filters or fluorescers
b. grazing incidence mirrors
c. transmission gratings
d. x-ray diodes or photocathodes.

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Reduction of data from x-ray instrumentation involves unfolding of source strength from the diagnostic output (charge, voltage pulse, and film density distribution). The unfolding process involves calculation of the response function which depends on mirror reflectivity, filter transmission, grating efficiency, x-ray diode and photocathode efficiency, etc. These quantities can be measured at a few x-ray energies but unfolding requires that they be defined on a fine photon energy grid. This can be accomplished by calculating component response with fitting to the measured data. To make these calculations, an extensive library of x-ray cross section and atomic scattering factor is needed in conjunction with software to calculate channel component responses. In this paper, we will describe the setup of one of these libraries and the associated software. The library and software was created for use on a VAX computer with the VMS operating system and a FORTRAN 77 compiler. The data library and associated software will be made available for distribution on magnetic tape. Requests for the library can be made to the authors.

## SETUP OF THE ATOMIC SCATTERING FACTOR LIBRARY

Several x-ray cross section libraries have been available for use at LLNL but none has provided the data in a form needed for the rapid calculation of reflectivity. To solve this need and to provide a data for x-ray channel response in the 0.1-10 keV range, a data base of atomic scattering factors $f_1$, $f_2$ was created in a keyed access file. The data base contains for each element from hydrogen to plutonium (HH to Pu) 294 discrete values of energy $f_1$, $f_2$ for an energy range of 0.1 to 10 keV.

The atomic scattering factor of $f_2$ is proportional to $E\mu_{pe}(E)$ where $\mu pe(E)$ is the photoelectric cross section. $f_1$ must be calculated from the integral:

$$f_1 = Z + C \int_0^{\infty} \frac{E'^2 \mu pe(E') dE'}{E^2 - E'^2} \qquad (1)$$

$f_1$ and $f_2$ values were both taken from existing sources (Reference 1) or calculated using the data of Reference 2. C is given by:

$$C = 1/\pi r_0 hc \qquad (2)$$

where $r_0$ = classical electron radius; h = planck's constant; c = speed of light. $f_2$ is calculated from the photoelectric cross section by:

$$f_2 = \pi/2\ CE\mu_{pe}(E) \qquad (3)$$

Reference 1 provided $f_1$ and $f_2$ values from 0.1 to 1.5 keV. These were incorporated directly into our library. Next a file of Biggs-Lighthill cross-section coefficients (Reference 2) was created on our VAX. Data was organized by element atomic symbol and the energy range for which each set of coefficients is defined. For a given element and energy zone n, the absorption cross section is defined in terms of the coefficients by:

$$\mu_{pe}(E) = \frac{An}{E} + \frac{Bn}{E^2} + \frac{Cn}{E^3} + \frac{Dn}{E^4} \qquad (4)$$

In performing the integration for $f_1$, cross section values μpe(E) were calculated from the $f_2$ values of Reference 1 from energies of 0.1 keV to 1.5 keV. From 1.5 keV to 10.0 keV, the Biggs-Lighthill coefficients were used. A numerical integration was carried out for energies less than 1.5 keV, but for energies > 1.5 keV, an exact integration of Equation 1 could be made for Equation (1) with $\mu_{pe}(E)$ of the form of Equation (4). The upper limit of integration was set at 85 keV to be consistent with Reference 1. It is to be noted that for the high Z elements, the integral will be larger for higher upper limits. For the low Z elements, the contribution of the $f_1$ integral above 85 keV is negligible. Figures 2, 3, and 4 show the results of calculations for elements of widely differing Z.

The library file on the VAX was designed for the quickest mode of access for the data desired. Scattering factor data is normally used in response functions as a set of data for a range of energies for a single material or element. This requirement is easily satisfied by writing the library in a keyed access file in which each record contains the $f_1$, $f_2$ data for a single element and the record key is the atomic symbol. Each record contains in binary form the following data:

Element atomic symbol
Atomic number
Atomic weight
Proportionality constant between $f_2$ and $E\mu pe(E)$
Proportionality constant between $\mu$(barns/atom) and $\mu$($cm^2$/gm)
284 values of energy for which $f_1$ and $f_2$ are calculated
284 values of $f_1$
284 values of $f_2$

The size of the keyed-access binary file containing the $f_1$, $f_2$ data is 600,000 bytes. The corresponding data written in ASCII requires roughly 1.5 megabytes of storage. One subroutine is needed to access the library: input is simply the atomic symbol; output is the $f_1$, $f_2$ and other values given above stored in memory. Time required to read a record of the keyed access file and store in memory is a small fraction of a second whereas it would take many tens of seconds to read the same data out of the file in ASCII format (which must be accessed sequentially).

## APPLICATIONS OF THE LIBRARY

The library is used as a data source in many codes for calculating responses of different x-ray diagnostics systems. As an example, we will describe a VAX based channel design code named FOIL which allows a user to calculate the response of an x-ray diagnostic consisting of an arbitrary numbers of filters and mirrors, photocathodes or x-ray diodes. All components can have their contribution to the total response calculated when the calculations are matched to measurements through various fitting parameters.

Separate software modules to calculate the response of each component were written and received component characteristics from the main module. As shown in Figure 5, the user enters material composition, geometry, and other parameters to define each component. For example, a mirror reflectivity calculation involves specification of the mirrors composition and grazing angle of the x-rays. A foil filter transmission calculation requires specification of thickness and material composition. Each component calculation subroutine or procedure calls the subroutine for extracting $f_1$, $f_2$ data out of the library. An extraction is made for each element specified in the material composition. The $f_1$, $f_2$ data is redefined at the energy values specified for the response calculation from the energy grid in the library file using log-log interpolation. After all components are specified, the response of each is calculated and then multiplied to give the total response (Figure 6). Figures 7 and 8 show some sample calculations for a KB x-ray microscope channel response and a broad band spectrometer channel response.

In addition to an interactive code for channel design, we also use the $f_1$, $f_2$ library to automatically calculate channel responses for which components are stored in a relational data base. This system is used for highly automated processing of broad-band spectrometer data.

## REFERENCES


1. B. Henke, P. Lee, T. Tanaka, R. Shimabukuro, B. Fujikawa, "Low-Energy X-Ray Interaction Coefficients Scattering and Reflection," Atomic Data and Nuclear Tables 27 (January 1982).

2. F. Biggs and R. Lighthill, "Analytical Approximations for X-Ray Cross Sections II," Sandia Report SC-RR-71 0507 (May 1982).

# X-Ray detector channel configuration

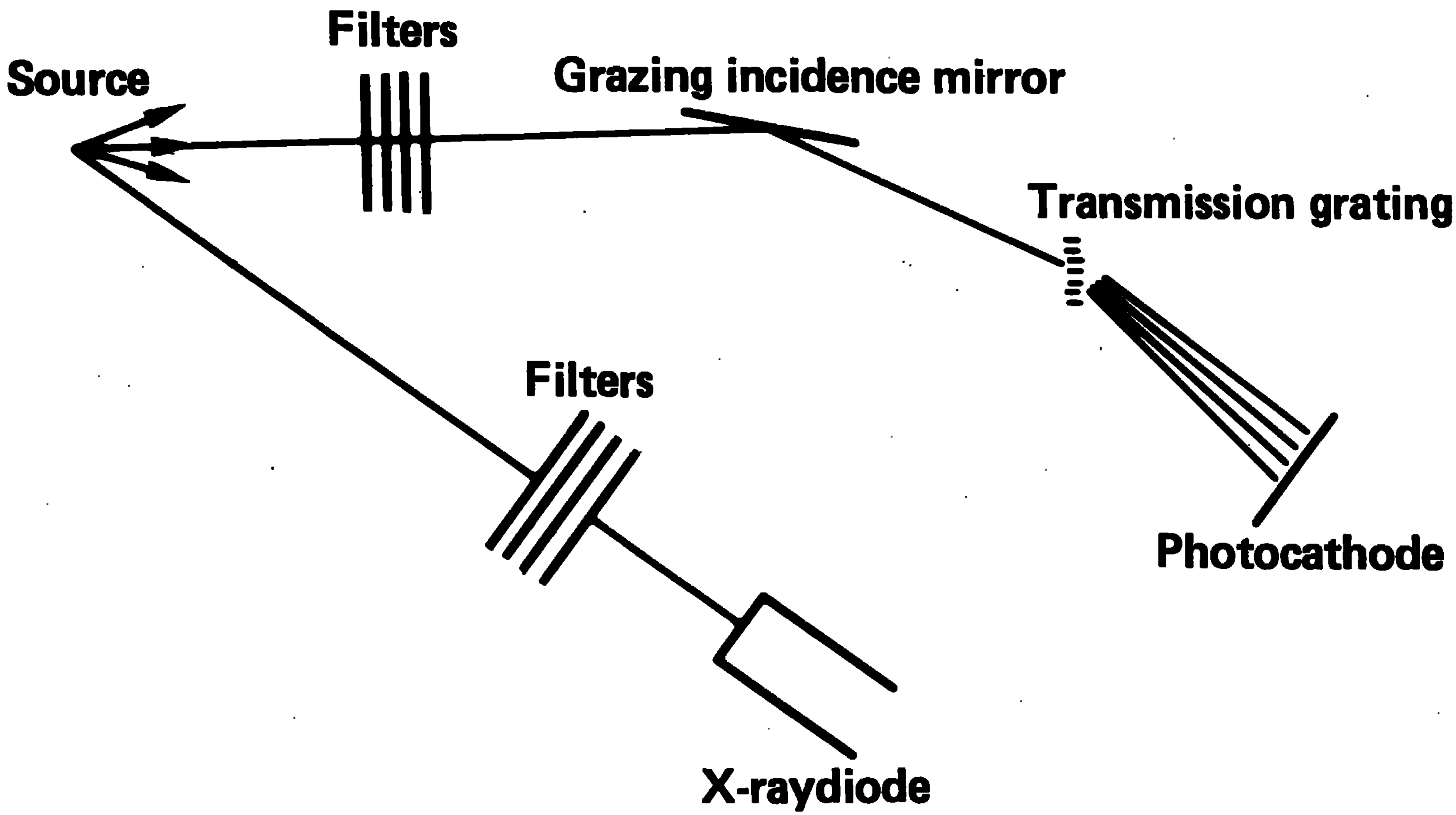


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Fig. 1

## Calculated f1 values for magnesium (Mg)

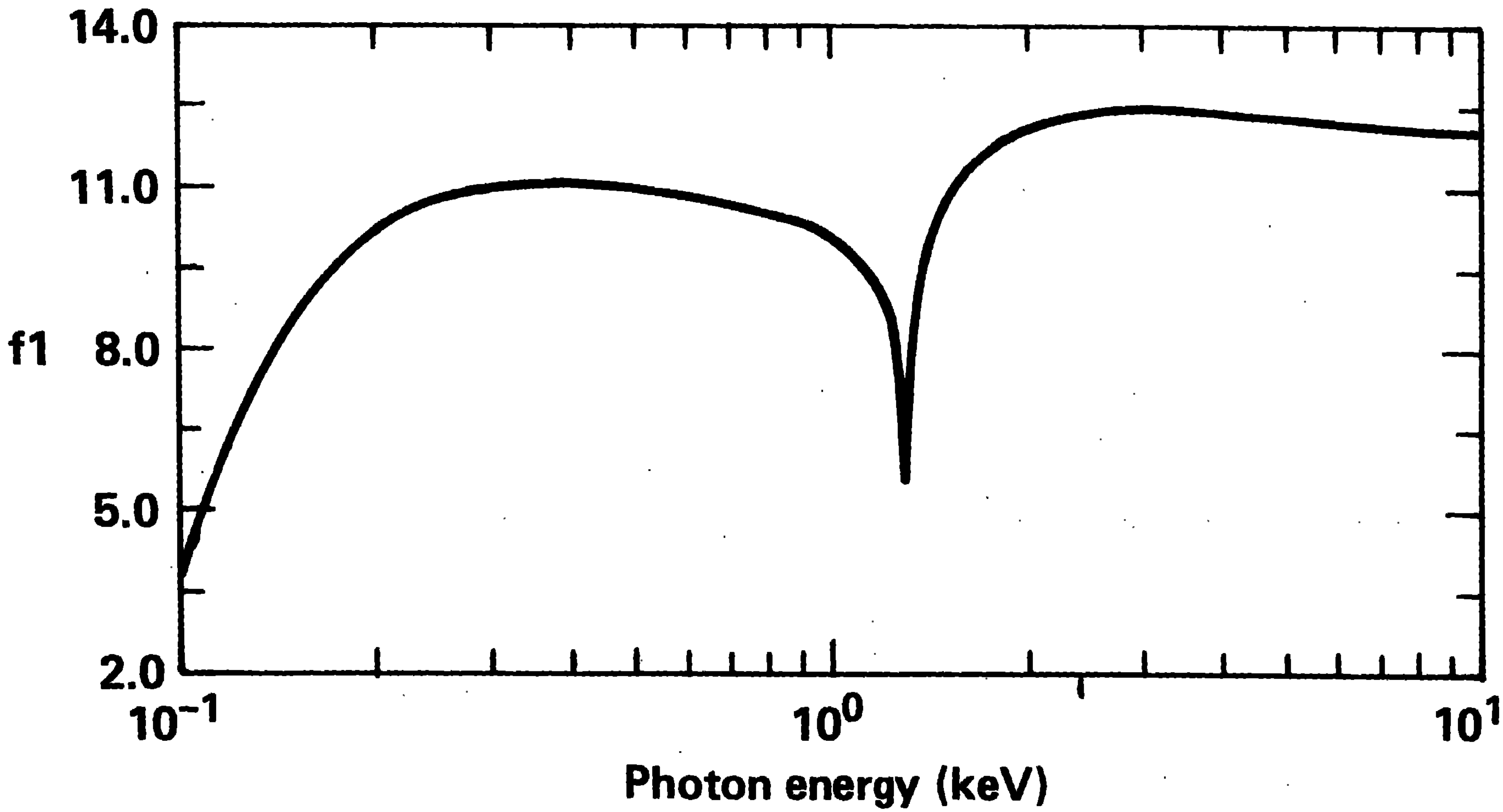
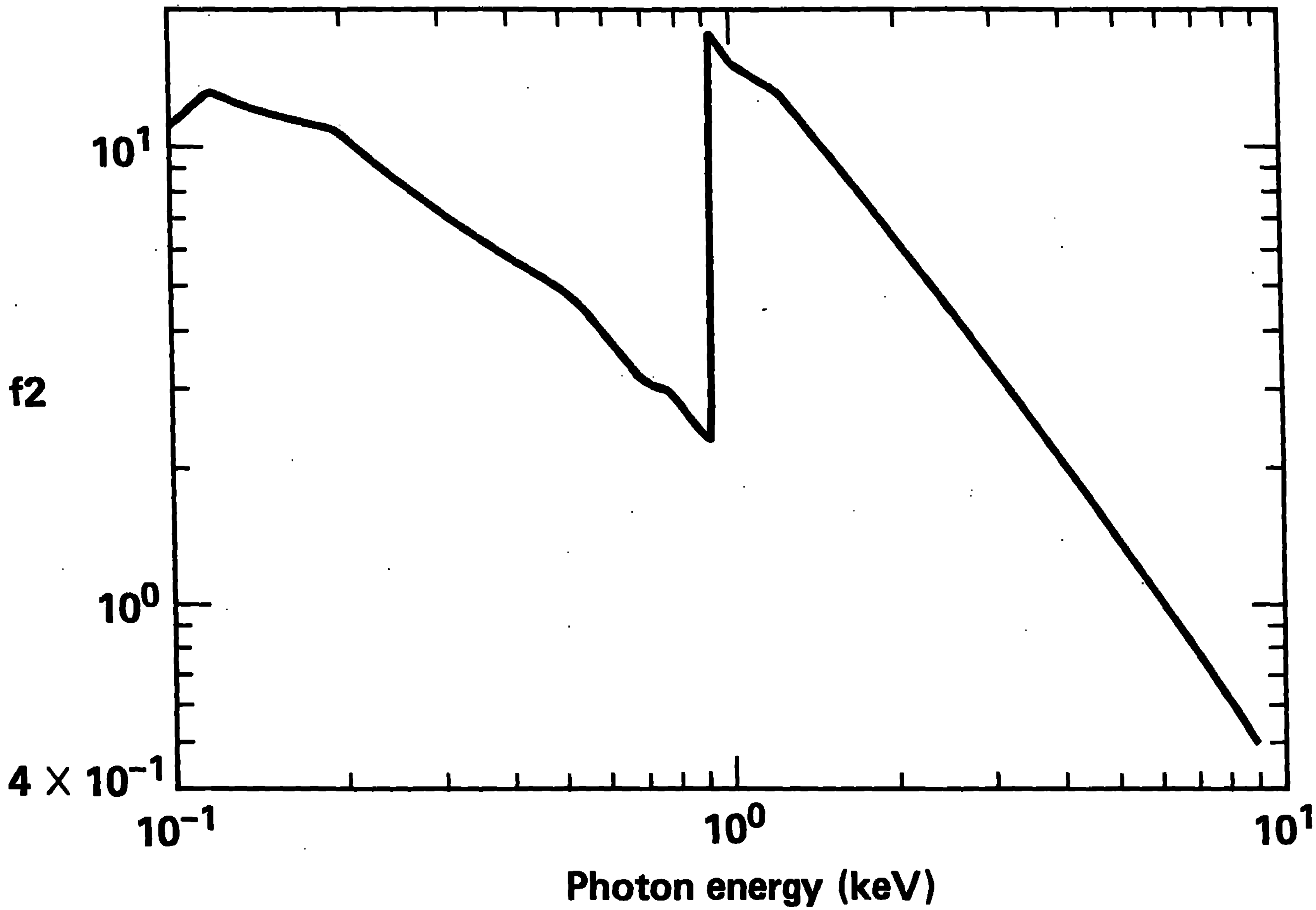



Fig. 2

# Calculated f2 values for copper (Cu)




20-01-1184-4547

Fig. 3

# Calculated f1 values for gold (Au)

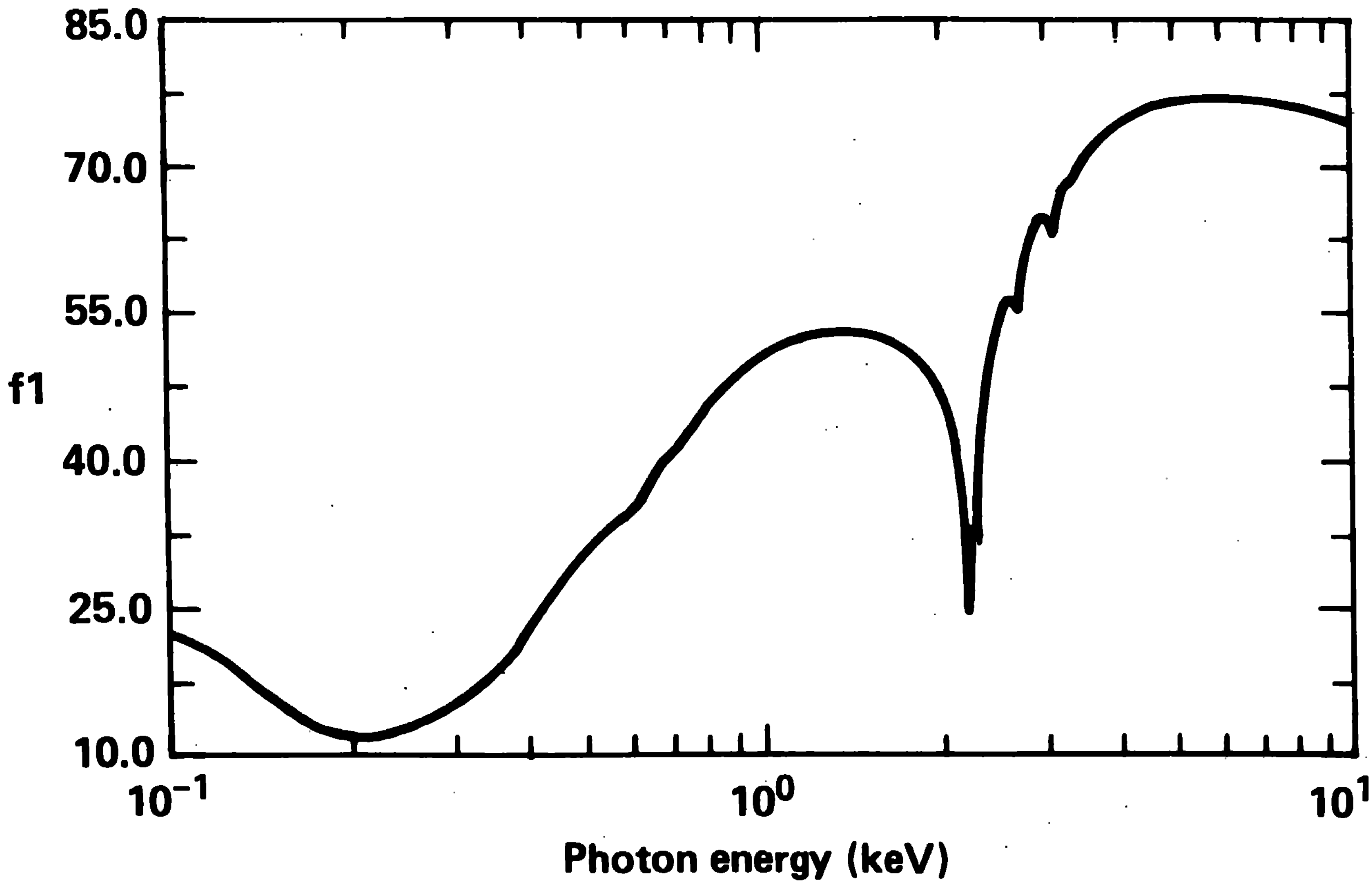



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Fig. 4

# Response function calculation software

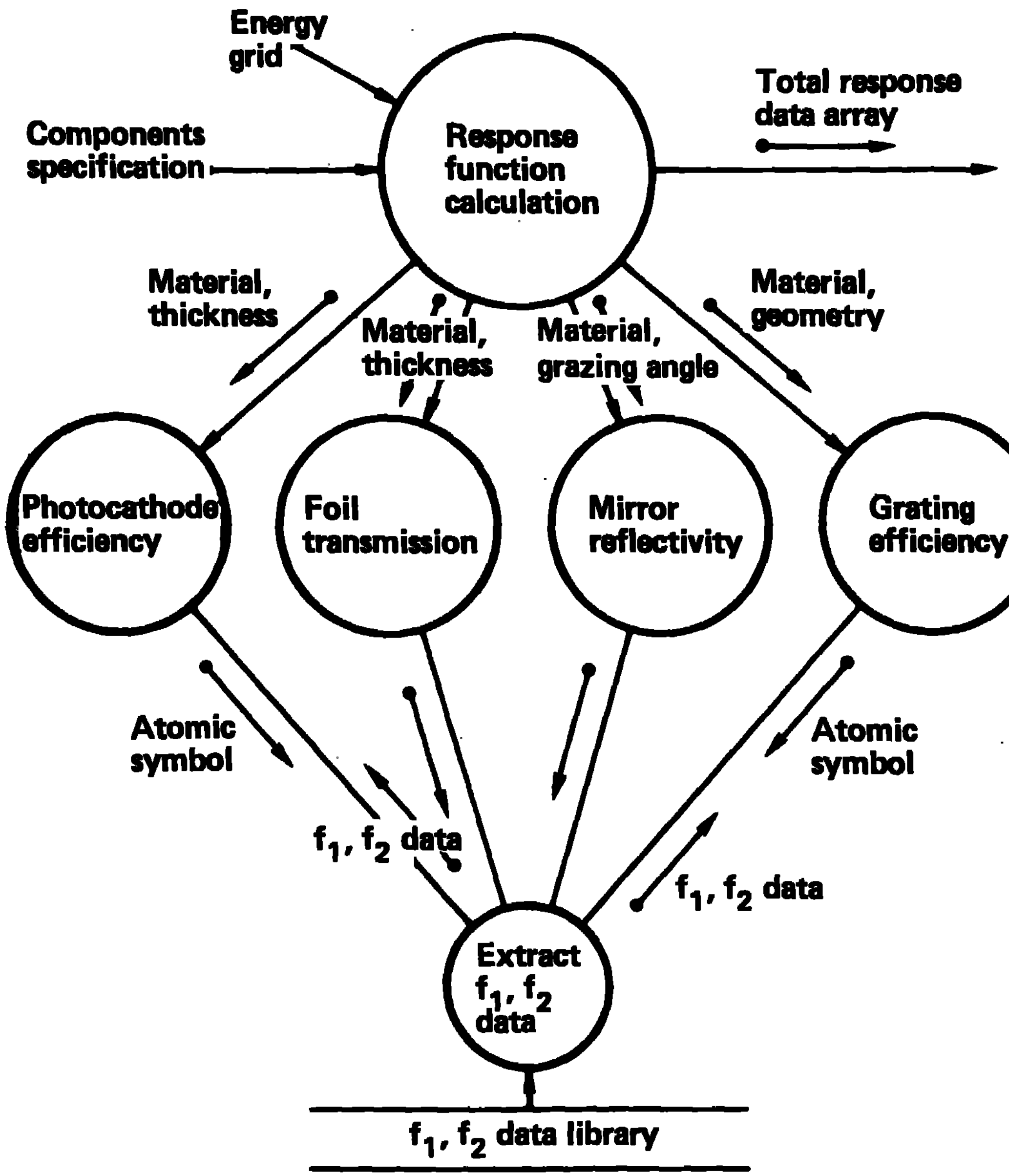


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Fig. 5

# Response function calculation

$$F(E) = \prod_{i=1}^{M} T_i(E) \quad * \quad \prod_{j=1}^{N} R_j(E) \quad * \quad GR(E) \quad * \quad S(E)$$

| Foil transmission | Mirror reflectivity | Grating efficiency | Active element sensitivity |
|---|---|---|---|

Fig. 6

# KB x-ray microscope channel response function

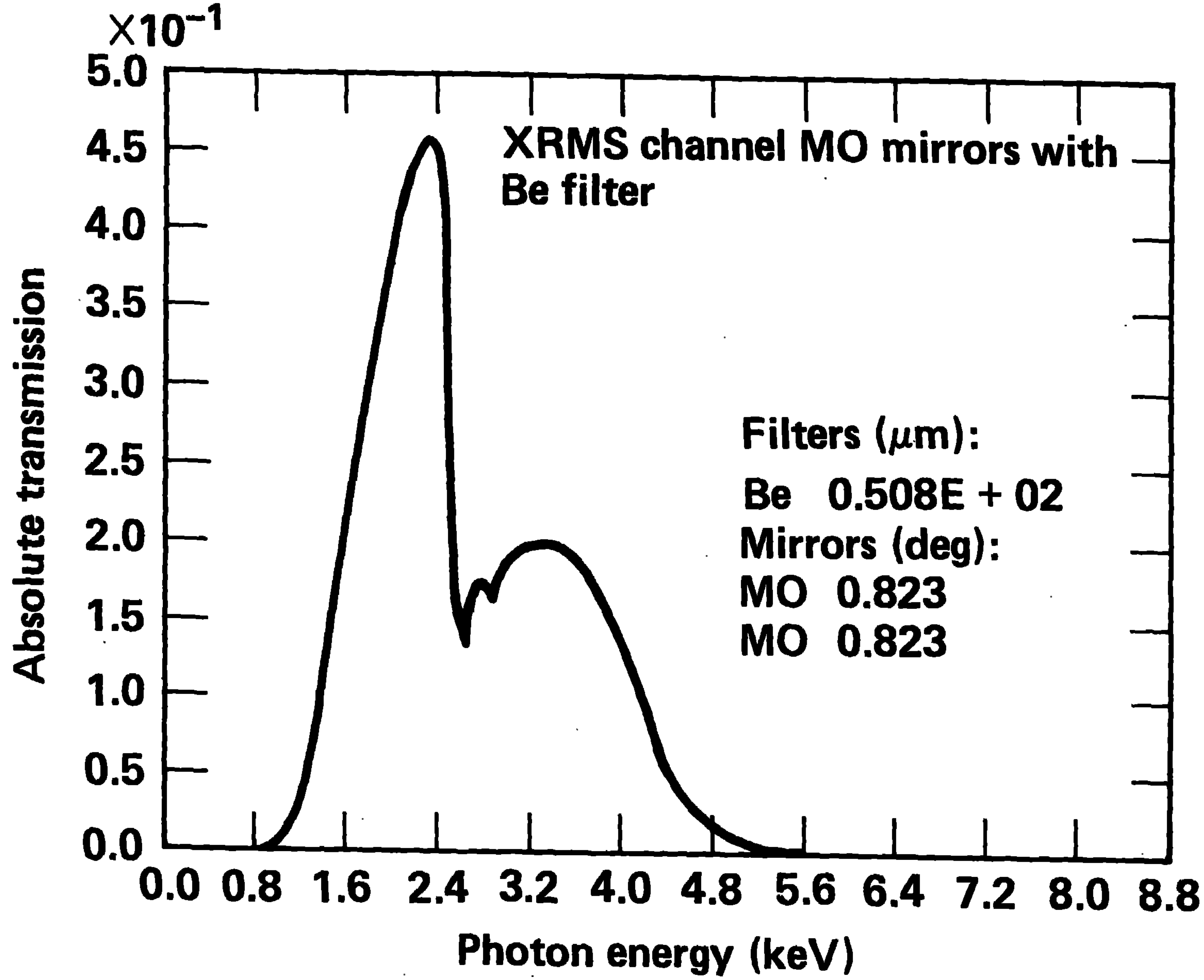


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Fig. 7

# Dante broad band spectrometer response function

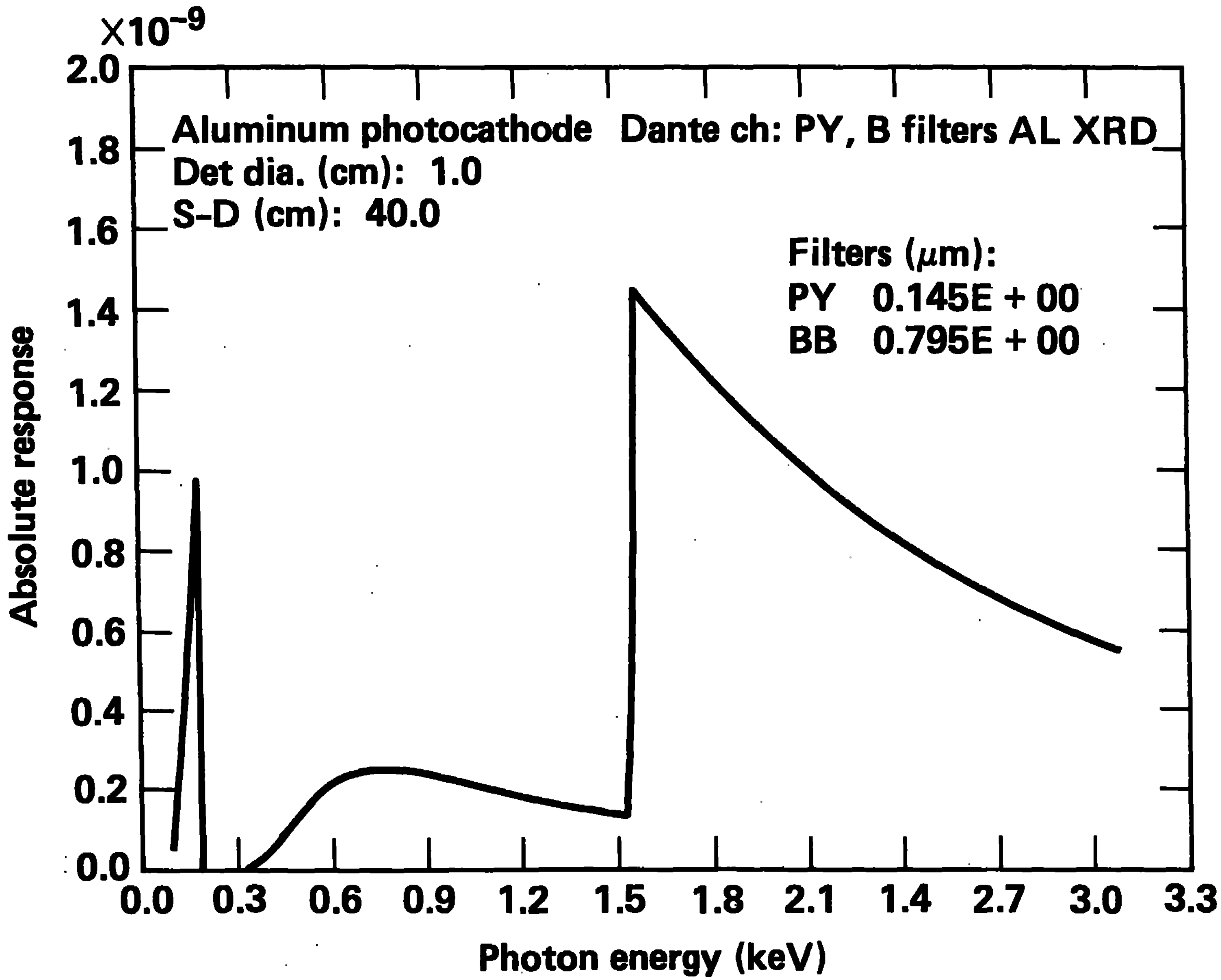


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Fig. 8